

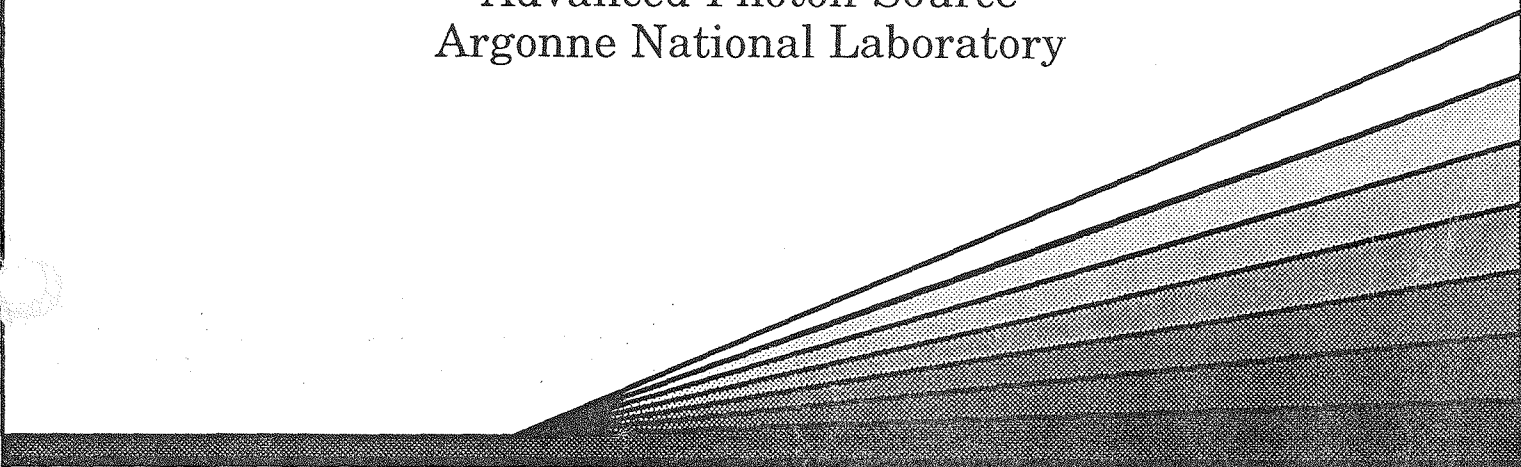
Diamond Monochromator for High Heat Flux Synchrotron X-ray Beams

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ABSTRACT

Single crystal silicon has been the material of choice for x-ray monochromators for the past several decades. However, the need for suitable monochromators to handle the high heat load of the next generation synchrotron x-ray beams on the one hand and the rapid and on-going advances in synthetic diamond technology on the other make a compelling case for the consideration of a diamond monochromator system. In this paper, we consider various aspects, advantages and disadvantages, and promises and pitfalls of such a system and evaluate the comparative performance of a diamond monochromator subjected to the high heat load of the most powerful x-ray beam that will become available in the next few years. The results of experiments performed to evaluate the diffraction properties of a currently available synthetic single crystal diamond are also presented. Fabrication of a diamond-based monochromator is within present technical means.

1. INTRODUCTION

The combination of high power and high power density associated with the x-ray beams generated by insertion devices at the third generation synchrotron radiation facilities has created new challenges in the design of the beamline components that intercept the x-ray beams. The challenge is nowhere greater than in the design of the first optical components, notably monochromators and mirrors, which must provide acceptable performance under the thermal load of the x-ray beams.

A resurgence of research activities in the development of monochromators for high heat load beamlines has led to examination of many aspects of the problem. Much attention has been concentrated on the cooling of monochromators with the aim to reduce the temperature gradient and thus the thermal distortion in the system.¹ Novel monochromator designs such as the inclined²⁻³ or asymmetric⁴ monochromator have also been suggested. The combined effort has resulted in the design of monochromators that can adequately handle the needs of the synchrotron community for the near future. For the x-ray beams that come on line in the second half of the decade, the currently available designs may not be adequate.

One area with substantial potential in the design of high performance monochromators is the monochromator material selection. In this paper, we consider this aspect of the problem and specifically suggest diamond as a material of choice. While diamond has previously been used in diffraction work, in this paper we consider its application in high heat load monochromators and provide a preliminary study of the design, fabrication, analysis, and characterization aspects of a diamond monochromator system.

2. MONOCHROMATOR MATERIAL

Currently, silicon is almost universally used in the design of monochromator systems for high energy (over 2-3 keV) x-ray beams. The choice arises from the availability of low-cost, large-size, and extremely high quality single crystal silicon developed primarily for the semiconductor industry. Single crystal diamonds have not been used for this application for a number of reasons. The two main (and mutually reinforcing) reasons have been a general lack of need for, and unavailability of, suitable single crystal diamonds for x-ray optics applications.

There are now some compelling reasons why the subject of a diamond monochromator should be reassessed. To begin with, the x-ray beams produced by undulators at modern synchrotron facilities are so intense that they cause unacceptably high thermal distortion in the cooled optical elements on which they impinge. Thus, an optically suitable single crystal with high thermal conductivity and low thermal expansion coefficient is highly desirable. Single crystal diamond *at room temperature* fits this description rather well as does silicon *at cryogenic temperatures*.^{5,6}

At temperatures below 20 K, single crystal silicon has a negligible thermal expansion coefficient, and its thermal conductivity is about 50 W/cm-K (i.e., about 12 times better than that of copper at room temperature).⁵ It has a negative thermal expansion coefficient below 125 K (i.e., it contracts upon heating). The thermal expansion coefficient is zero at about 125 K where the thermal conductivity is about 6 W/cm-K (or 50% better than that of copper at room temperature). Thus, a cryogenically cooled silicon monochromator system, operated for example at liquid nitrogen temperature, is conceptually attractive. In practice, however, the design of a system capable of removing several kW of heat with on-the-surface peak heat fluxes in excess of 50 W/mm² (expected from APS Undulator A, for example) is a rather formidable task, the most obvious complications of which are the critical heat flux issue, the required large cooling area that necessitates a multi-layer heat exchanger, and a robust design for maintaining the integrity and the figure under thermal cycling. It is more realistic to consider a cryogenically cooled silicon monochromator system with an inclined or asymmetric geometry in which the incident heat flux is spread out over a much larger area than in a conventional monochromator.²

Diamond at room temperature offers a more manageable and yet competitive alternative to silicon at cryogenic temperatures. Single crystal diamond can have a thermal conductivity in excess of 21 W/cm-K. This is five times better than copper at room temperature, and the ratio is accentuated at lower temperatures, to some 25 times at liquid air temperature (Type IIa diamond has a fantastic thermal conductivity of about 100 W/cm-K at about 100K). Thus, it is apparent that, at least from a thermal point of view, a diamond-based monochromator system can provide an option for dealing with high thermal load x-ray beams.

In using diamond for the design of an x-ray monochromator system, however, a number of issues must first be resolved. These concern the availability, quality, and suitability of diamonds for synchrotron applications. These issues are discussed next.

3. SINGLE CRYSTAL DIAMONDS

Diamonds⁶⁻⁹ are classified (based on their IR and UV absorptions) as Type I or II depending on whether nitrogen, a common impurity, is present or not. Each Type is further subdivided into a or b, to indicate the specific form in which impurities are present. A majority of natural diamonds are Type I, with high concentrations of nitrogen, while Type II diamonds (which make up about 2% of diamonds) have

little or no nitrogen. Type II diamonds contain impurities with concentrations of about 10 parts per million and as gem stones are considered to be nearly "perfect" and free from "defects." Most of these are Type IIa, having a high electrical resistivity ($\sim 5 \times 10^{14}$ ohm-m), and are essentially insulators. Type IIb diamonds, on the other hand, are semiconductors with a resistivity of 100 ohm-m or less, due to the presence of boron as an impurity.

High quality natural diamonds are available in sizes up to $10 \times 10 \times 1 \text{ mm}^3$ or larger.¹⁰⁻¹¹ The current price¹⁰ for a $10 \times 10 \times 0.25 \text{ mm}^3$ Type IIa diamond is under \$8000. Larger area diamonds can be available at substantially higher costs. Type IIb crystal prices are about twice those of Type IIa diamonds. Type Ia diamonds are not suitable for the present application, while Type Ib diamonds, which are available in sizes up to $6 \text{ mm} \times 6 \text{ mm} \times 0.25 \text{ mm}$ (or thicker), are priced at about \$2000 or roughly about 20% higher than Type IIa diamonds of the same size.¹⁰

For x-ray diffraction applications, one may ideally want to use a perfect diamond crystal, that is a diamond free of all impurities and lattice defects & dislocations. Such crystals are rare, and extensive testing of many crystals is necessary to select a suitable specimen. We note, however, that certain imperfections in single crystal diamonds may even be desirable in certain x-ray diffraction applications.

A high quality diamond, in the aesthetic sense, with no "impurities" may still be (and often is) imperfect, in the diffraction sense. This is due to lattice defects and lattice deformations. The former include missing or displaced atoms from the points of their geometric location and local elastic deformations which alter the inter atomic spacing and the bond lengths. Lattice deformations are due to the presence of a few or a large number of elastically strained regions in the crystal leading to a crystal that is divided into many small regions with slightly different lattice orientations. This is the mosaicity of the single crystal diamond that broadens the rocking curve.

Natural diamonds are generally stressed. Sometimes a part of this stress may be annealed by heating the diamond in vacuum (to prevent oxidation) or by heating it to very high temperatures for a short period of time (to prevent graphitization.) in an inert environment

A rather unexpected result of a limited number of studies on the diffraction properties of natural diamonds is that because of a type of dislocation commonly found in and characteristic of the more "perfect" Type IIa diamonds, Type Ib diamonds are actually more suitable for x-ray monochromators.¹² To our knowledge, the only reported confirmation of this by precise rocking curve measurements is due to Jackson¹³ who obtained a double crystal rocking curve width (apparently the full width at half maximum, or FWHM) of about 150 arc seconds for a Type IIa diamond and only 10 arc seconds for a Type Ib diamond, both from (022) crystal planes. The photon energy is not specified, but the theoretical FWHM of the double crystal rocking curve calculated¹⁴ for these specimen ranges from 1.5 arc seconds for 20 keV to 32 arc seconds for 5 keV photons. Jackson¹³ also notes that the annealing of the Type IIa crystals to 1000°C failed to affect the rocking curve width.

Because of the recent availability of synthetic single crystal diamonds and our belief that the rapid advances in diamond technology may soon result in larger area diamonds of high consistency and quality, we have examined Type Ib synthetic crystals produced by Sumitomo Electric.¹⁵ These crystals known as Sumicrystals™, are about $5 \times 5 \times 0.3 \text{ mm}^3$ in size and are developed primarily as a heat sink material. They have a yellow color, indicative of nitrogen impurity, which is reported by the manufacturer to be on the order of tens of parts per million. The crystals are cut, using a Yag laser beam, from larger crystals that are synthesized in a high pressure (about 50,000 atmospheres) and high temperature (over 1300°C) process. The Sumicrystals™ have not, to our knowledge, been adequately characterized for x-ray

applications, although there are indications that they may be better than most natural diamonds in crystalline quality and in consistency.

The high pressure-high temperature technique to produce synthetic diamond crystals (first announced by the General Electric (GE) researchers in 1955 and detailed later,¹⁶) has been modified and refined to produce larger and higher quality single crystal diamonds. The only single crystal diamonds that General Electric now supplies are the isotropically pure (99.99%) C¹² crystals.¹⁷ Owing to the much reduced irregularities in the crystal lattice vibrations present in diamonds with natural isotropic composition, the GE crystals have a room temperature thermal conductivity of 33 W/cm²-K, or 50% above that of the best natural diamonds. Two (400) GE samples (4 mm x 4 mm in area) evaluated on the X-25 beamline at Brookhaven National Laboratory¹⁸ using a (440) silicon analyzer gave rocking curve FWHMs of 2.5 and 8 arc seconds, confirming that at least one of the two is an extremely good crystal. Other investigations show that the rocking curve widths for these crystals are not perceptively dependent on the isotropic composition.¹⁹ The size of GE crystals, according to the supplier, does not exceed 5 mm x 5 mm in area.¹⁷

During the course of the present study, it has become obvious that the potential x-ray optical applications of synthetic diamonds have not been communicated to the respective manufactures. In fact, the SumicrystalsTM diamonds that we have examined are mostly used for heat sink applications, and have not benefited from any special handling (in cutting, polishing, etc.) appropriate for optical applications. We have measured the RMS surface roughness of these diamond crystals to be about 10Å with a radius of curvature of about 10 m. The largest synthetic diamond crystals currently available¹⁵ from Sumitomo is about 12 x 12 x 0.3 mm³ and costs about \$32,000. An 8 x 12 x 0.3 mm³ costs about \$19,000. As we shall shortly see, these sizes are adequate for the present application.

4. ROCKING CURVE MEASUREMENTS

Two SumicrystalTM diamond specimens, 5 x 5 x 0.3 mm³ in size, were first tested using a Laue camera to determine the crystal planes. The large surface area of the crystals were found to be nearly parallel to the (400) planes. These planes were used in the Bragg diffraction experiments to determine the quality of the synthetic crystals. The experimental setup for these experiments is shown in Fig. 1. The radiation from a Mo-K x-ray source (on the right) passes through a set of double (vertical and horizontal) slits and impinges on the first diamond crystal. The diffracted beam from this crystal passes through a second set of double slits and impinges on the second crystal where the radiation is diffracted for a second time. The intensity of this diffracted beam is recorded with the x-ray detector on the left. This is the standard non-dispersive geometry used to determine the average quality of two crystals. The horizontal widths of the first and second slits are 0.025 mm and 0.15 mm, respectively. These are sufficient to limit the diffraction to one of the K x-ray lines (K α 1) in the Mo spectrum. The footprint of the beam on the second crystal is about 0.6 mm horizontally and 3.0 mm vertically. The double crystal rocking curve (photon count rate as a function of Bragg angle) is obtained by rotating the second crystal and recording the photon count rate.

The set up shown in Fig. 1 was first tested by measuring the double crystal rocking curve FWHMs of nearly perfect silicon (111) and (333) crystals. Values of 4.8 and 0.96 arc seconds, respectively, were obtained, which when divided by $\sqrt{2}$ give the corresponding average widths of individual crystals as 3.38 and 0.68 arc seconds. These values are accurate to better than 3% when compared to the theoretical values (Darwin widths) of 3.32 and 0.66 arc seconds, respectively.

The double crystal rocking curve of diamond (400) crystals was then obtained as shown in Fig. 2. Also shown in Fig. 2 for comparison is the rocking curve obtained by replacing the diamonds with silicon (111) crystals *without* changing the photon source or the slit sizes. The measured double crystal rocking curve FWHM for diamond (400) is 6.2 arc seconds and for silicon (111) is 4.8 arc seconds. If the diamond crystals were perfect, one would expect to obtain¹⁴ a rocking curve with a FWHM of 0.97 arc seconds as shown in Fig. 3. Thus, most of the measured line width in the diamond is related to the crystal imperfections. The measured average width of a Sumicrystal™ is then $6.2/\sqrt{2}=4.4$ arc seconds, while a perfect diamond (400) would have a FWHM (Darwin width) of $0.97/\sqrt{2}=0.69$ arc seconds.

With the above information, it is possible to estimate the average mosaic width of the diamond crystals. Assuming that the mosaic width adds to the Darwin width as the square root of the sum of the squares, the mosaic width will be given by the square root of the difference between the squares of the measured and theoretical (Darwin) widths, that is,

$$\text{Mosaic width} = \left[4.4^2 - 0.69^2 \right]^{1/2} = 4.35 \text{ arc seconds}$$

Assuming that the mosaicity is isotropic, one can now use this value of the mosaic width to estimate the FWHM of these diamond crystals when they are used to diffract x-rays, for example, from the (111) planes. One combines the theoretical diamond (400) width of 3.1 arc seconds with the mosaic width of 4.35 arc seconds to obtain the value of 5.3 arc seconds for this width. Thus a two crystal monochromator system using these diamond crystals with the (111) planes should generate a rocking curve with a FWHM of $5.3\sqrt{2}$, or 7.5 arc seconds. The results of the rocking curve experiments are summarized in Table I.

Table I. Results of the rocking curve experiments with diamond and silicon crystals. All experiments were performed with the Mo K α 1 x-ray. Given widths are all for one crystal.

Description	width (arc seconds)
Measured average width of the synthetic (400) diamond specimens	4.4
Theoretical (Darwin) width of a perfect (400) diamond crystal	0.69
Estimated mosaic width of the synthetic diamond specimens	4.35
Estimated width of the synthetic (111) diamond crystal*	5.3

*denotes inferred values based on the computed mosaicity.

The diamond rocking curve (shown in Fig. 2 as a solid line with data points) taken with two diamond crystals, used the same experimental setup and source intensity that was used to obtain the silicon rocking curve (dashed curve) from two perfect silicon crystals. What is of special interest here is that not only the two rocking curve widths but also their peak intensities are quite similar. If diamond crystals of this quality were used in a double crystal monochromator both the opening angle of the diffracted beam (which is a function of the width of the rocking curve and the opening angle of the synchrotron beam) and the peak counting rate in the diffracted beam would be quite similar.

The main difference between such diamond (400) and the silicon (111) double crystal monochromators is that the Bragg angle for the diamond case is a factor of 3.6 larger than the Bragg angle used in the silicon monochromator when diffracting the same energy x-ray. This will narrow the width of the energy band diffracted by the diamond monochromator by a similar factor of 3.6 since $\Delta E/E$ is

proportional to $\Delta\theta/\theta$ where $\Delta\theta$ is the opening angle of the diffracted beam (similar for both cases), and θ is the Bragg diffraction angle which is 3.6 times larger for the diamond case. If the peak intensities are similar as the experiments suggest, then there will be 3.6 times as many photons per unit bandwidth in the diffracted beam of the diamond monochromator. The integrated diffraction efficiency for the (111) diamond planes is expected to be larger than for the (400) planes, so that diamond (111) planes will produce monochromators with even higher intensities in the diffracted beam.

5. FABRICATION OF A DIAMOND MONOCHROMATOR

Although single crystal diamonds currently available are rather modest in size, they are adequate for the collimated high power density x-ray beams generated by undulators. A $12 \times 8 \text{ mm}^2$ diamond is large enough to intercept the central cone of the APS Undulator A.^{2,20} At 30 m from the source, the central cone of the x-ray beam at closed gap (at which the power loading is maximum) is about 3.6 mm horizontally and 1.2 mm vertically (full width at zero height). This means that a (111) diamond crystal, 12 mm long, can intercept and diffract the entire central cone radiation at Bragg angles of 5.7° or larger. This covers the entire 4-30 keV tuning range of Undulator A. Small(er) Bragg angles corresponding to high(er) diffracted photon energies require tuning the undulator to higher harmonic energies at which the power loading of the beam is substantially reduced and therefore a silicon monochromator can be used.

Because of its low atomic number, diamond absorbs less x-ray radiation than does silicon of identical thickness. The PHOTON²¹ program was used to calculate the absorbed values. The results are shown in Fig. 4 for APS Undulator A (see specifications in Table II). The thickness of the diffracting diamond can be as small as tens of microns. The thinner the diamond, the less the absorbed radiation, and therefore the smaller the thermal load on it. It is thus advantageous to use a thin diamond monochromator if the crystal can be convectively surface-cooled, for example, by a helium or nitrogen jet. If the crystal is edge cooled, then the thinner the crystal, the smaller is the conduction area for the transfer of the heat from the center of the crystal to its cooled periphery, and the net effect on the temperature and strain in the crystal is, in general, insignificant. The important parameter in edge cooling is the effective heat transfer coefficient at the crystal boundaries. Because of the high conductivity of diamond, a doubling of the effective heat transfer coefficient at the crystal edges will reduce the maximum temperature in the crystal nearly by half. Thus, a thin crystal with edge cooling may be an option depending on the absorbed heat load and the edge cooling efficiency. For the APS Undulator A beam considered in this study, we assume that the diffracting single crystal diamond is bonded to a substrate made of polycrystalline diamond to build what we call an integral diamond crystal. Polycrystalline diamonds can have high thermal conductivities²² approaching that of single crystal diamonds and, more importantly, they can be produced in large sizes using chemical vapor deposition (CVD) or associated techniques. The diamond (or possibly silicon) diffracting element can be bonded²³ to a CVD substrate with appropriately configured cooling channels. With a carefully selected bonding procedure, one may be able to produce strain-free diamond to diamond bonding. We are unaware of any work in which the stress levels in such bonding were measured. An alternative technique would involve deposition of CVD diamond directly on the diffracting diamond element. Again, we are unaware of any work to produce or test stain-free bonding using this technique but believe that this may not be an insurmountable problem.

6. THERMAL AND STRUCTURAL ASPECTS OF AN INTEGRAL DIAMOND MONOCHROMATOR

In order to determine the relative performance of a diamond-based versus a silicon-based monochromator system, the slope errors resulting from the thermal distortion of the monochromators under the high heat load of an x-ray beam are required. As a rule of thumb, a figure of merit for the

performance is given by the ratio k/α , where k is the thermal conductivity and α is the thermal expansion coefficient. As seen from the property data in Table II, single crystal diamond can have a figure of merit 40 to 50 times higher than silicon at room temperature. The thermal conductivity of polycrystalline diamond is in the 7-21 W/cm²-K range (and possibly higher).²² Its thermal expansion coefficient is similar to that of single crystal diamond.

Table II. Properties of single crystal diamond and silicon at room temperature.⁶⁻⁹

Property	Diamond	Silicon
Atomic number, Z	6	14
Density (g/cm ³)	3.516	2.330
Thermal conductivity (W/cm-K)	21	1.25
Thermal expansion coefficient (K ⁻¹ x 10 ⁻⁶)	0.8	2.33
Specific heat (J/Kg-K)	520	750
Thermal diffusivity (cm ² /s)	11.5	0.72
Young's modules (GPa)	1,050	167
Poisons ratio	0.1-0.29	0.3
Melting point (°C)	4300	1420
Tensile strength (GPa)	>3	NA
Yield strength (MPa)	NA	1240-2060
Lattice spacing (Å)	3.5670	5.4305

For a more detailed comparison of the performances, we evaluate the temperature fields and the resulting slope errors in the two monochromator systems, one silicon and the other diamond. The radiation source is assumed to be Undulator A at closed gap (11.5 mm) on the 7-GeV APS storage ring with a positron current of 100 mA. The total power of the source is 3.8 kW, and the peak normal incidence heat flux at the monochromator 30 m from the center of the undulator is about 150 W/mm². The FWHMs of the beam in the horizontal and vertical directions are 8.2 and 2.9 mm, respectively. The central cone of the beam, which contains most of the desired (harmonic) photons, has a much smaller footprint. For APS Undulator A at 30 m from the source, the entire (full width at zero height) central cone has a footprint of 3.6 mm horizontally and 1.2 mm vertically.

In the computations that follow, it is assumed that an aperture with an opening of 3.6 mm and 1.8 mm in the horizontal and vertical directions, respectively, is placed upstream of the monochromator. Note that the vertical dimension of this slit is 50% larger than the 1.2 mm of the beam central cone.

It is also assumed that the entire heat load intercepted by the monochromator is absorbed on the surface, an assumption that is more appropriate for silicon than for diamond. In fact, as shown in Fig. 4, for APS Undulator A with a characteristic energy of 23.5 keV, about 30% of the power is absorbed in a 1 mm thick diamond. This figure for silicon is about 50%. In-depth absorption of heat will generally lead to reduced temperatures and strains. As mentioned previously, the low absorption of hard x-rays in diamond favors the possible use of a thin single crystal diamond in Bragg or Laue geometries. For example, for typical incident angles greater than 5°, a 0.2 mm diamond set to diffract Undulator A beam will absorb no more than 35% of the incident beam power. Note that the actual beam path length in the 0.2 mm thick foil is 2.2 mm. It may be possible to edge cool the thin diamond. The cooling, as we have noted, would have to be exceptionally good to maintain moderate temperatures and strains in the diamond.

In the present study, the total power intercepted by the monochromator through the aforementioned aperture is 860 W. We set the monochromators to diffract third harmonic radiation (12.6 keV) from Undulator A at closed gap. The crystals are assumed to be 1 cm thick. The widths and lengths are each 2 cm larger than the corresponding dimensions of the beam footprint. The thickness of 1 cm is arbitrarily chosen *for comparison only*, and, in fact, it is neither necessary nor optimal to have such thick substrates. The substrates are assumed to be cooled on the back surface by liquid gallium. The heat transfer coefficient used is 5 W/cm²-K. Again, this value is somewhat arbitrary but sufficient for the present comparative study. Table III summarizes these input data.

Table III. Parameters and data used in thermal and structural analyses.

Parameter	Data
Radiation Source	2.5 m Undulator A (closed gap)
Beam current	100 mA
Total power	3.8 kW
Power density	135 kW/mrad ²
Beam V-FWHM @30 m	2.9 mm
Beam H-FWHM @30 m	8.1 mm
Thermal Slit Location	30 m from the source
Slit opening (v x h)	1.8 x 3.6 mm
Beam footprint (v x h)	7.5 mm x 3.6 mm
Absorbed radiation	surface absorption assumed
Monochromator	diamond or silicon
Monochromator location	30 m from the source
Cooling (on back surface)	gallium
Heat transfer coefficient	5 W/cm ² -K
Total power intercepted	860 W
Peak normal incident heat flux	150 W/mm ²
Diffracting photon Energy	12.6 keV
Undulator harmonic	3rd

The model used in the thermal-structural analyses of the diamond monochromator is shown in Fig. 5. The dimensions of the beam footprints and the monochromator components are given in Table III. The thickness of the single crystal diamond (assumed to have been bonded onto the substrate) is 0.5 mm, which is more than sufficient for diffraction purposes. In the case of silicon, the substrate is also the diffracting element. Because silicon has a relatively low thermal conductivity, we have also considered a silicon crystal, 0.1 cm thick, to show the effect of reducing substrate thickness.

The temperature profiles along the AA'-axis (Fig. 5) for the diamond and silicon monochromators with 1-cm substrates are shown in Fig 6. In the case of diamond, the temperature on the top surface of the diffracting element (the heavy line) is slightly above the top surface of the substrate (the light line). For the silicon case, they are the same surface and thus the same temperature. The footprint region, which is smaller for the diamond monochromator (larger Bragg angle), is highlighted by the thicker line in Fig. 6. The maximum temperature rise in the silicon monochromator is about 660°C, while in the diamond monochromator it is about 55°C. A reduction in the thickness of the silicon monochromator from 1.0 cm to 0.1 cm will not lower the temperatures substantially (see Table IV).

Figure 7 shows the corresponding thermal distortions for the two monochromators. It plots the displacement in the plane of scattering along the length (A-A' in Fig. 5) of the crystal monochromators. The maximum displacements for silicon and diamond crystals are 0.27 μm and 14 μm , respectively. The displacement in a 0.1-cm-thick silicon crystal is not significantly different from that in a 1.0-cm-thick crystal. It should be noted, however, that this displacement would be substantially less if (as is normally the case) the crystal were restrained. The maximum temperature in the crystal is reduced by more efficient cooling, while the temperature gradient across the thickness, to a first approximation, remains unaffected.

Table IV. Simulation data and results for diamond and silicon monochromators.

Material	Diamond	Silicon	
Diffracting planes	(111)	(111)	
Photon energy (keV)	12.6	12.6	
Bragg angle ($^{\circ}$)	13.8	8.99	
Monochromator size (cm x cm)	4.7 x 2.2	6.6 x 2.2	
Beam footprint, v x h (cm x cm)	0.75 x 0.36	1.2 x 0.36	
Diffracting element size (cm x cm)	0.75 x 0.36	NA	
Diffracting element thickness (cm)	0.05	NA	
Peak incident heat flux (W/mm^2)	35	23	
Monochromator substrate thickness (cm)	1.0	1.0	0.1
Max. temperature rise above gallium temperature ($^{\circ}\text{C}$)	55	660	506
Max. temp. rise at wall-Ga interface ($^{\circ}\text{C}$)	18	27	280
Max. temp. rise across the crystal ($^{\circ}\text{C}$)	37	633	226
Max. compressive stress (MPa)	21	154	136
Max. tensile stress (MPa)	8	46	33
Max. displacement in the scattering plane (μm)	0.27	14	18
Max. slope error in the scattering plane (arc second)	5	180	200

The slope errors along the AA'-axis for the two 1-cm thick monochromators are shown in Fig. 8, where again, the footprint regions are highlighted. The maximum slope errors, which occur near periphery of the footprints, are about 5 arc second for diamond and 180 arc seconds for silicon. Since the photon beams have typically Gaussian profiles with their peaks where slope error is negligible and their nadir where the slope error is maximum, the *effective slope* errors are somewhat smaller.

7. SUMMARY AND CONCLUSIONS

We have proposed a diamond-based monochromator for very high heat load beamlines. The monochromator consists of a small single crystal diamond bonded to a polycrystalline diamond substrate in which the necessary cooling channels are configured.

A preliminary study of the subject examines the potential of such a monochromator. From a thermal-structural point of view, a diamond monochromator is vastly superior to a silicon monochromator. A simulated comparison of a silicon versus a diamond monochromator subjected to the APS Undulator A beam at closed gap indicates slope errors of 180 and 5 arc seconds, respectively. While the inclined monochromator^{2,3} provides a solution to the high heat load monochromator problem, a diamond monochromator allows conventional (non-inclined) operation of a monochromator. In addition, a diamond monochromator can be devised to operate in an inclined mode, in which case there is potential to

be able to handle heat fluxes *an order of magnitude higher* than those generated by undulators in the near future. This last statement assumes that one can obtain larger (2-4 cm size) single crystal diamonds.

Preliminary testing of Sumitomo synthetic single crystal diamonds, 5 mm x 5 mm x 0.3 mm, gave a double crystal rocking curve (for Mo $K\alpha_1$) of about 6 arc second compared to the theoretical value of about 1 arc second. These measurements must be carefully repeated. Further study and characterization of these crystals is necessary to evaluate their suitability as monochromator material.²⁴ It should also be realized that, unlike silicon, commercially available diamonds are restricted to a limited number of crystal orientations.

A number of additional issues must be investigated to determine the suitability of diamond as the monochromator material for routine use on high heat load synchrotron beamlines.²⁵ These include (a) strain-free bonding of diamond to diamond, or deposition of CVD diamond on the single crystal diffracting element, (b) dimensional stability of a composite diamond monochromator, (c) radiation damage study for diamond,²⁶⁻²⁸ and (d) further investigation of the diffraction properties of commercially available diamond crystals over large areas.

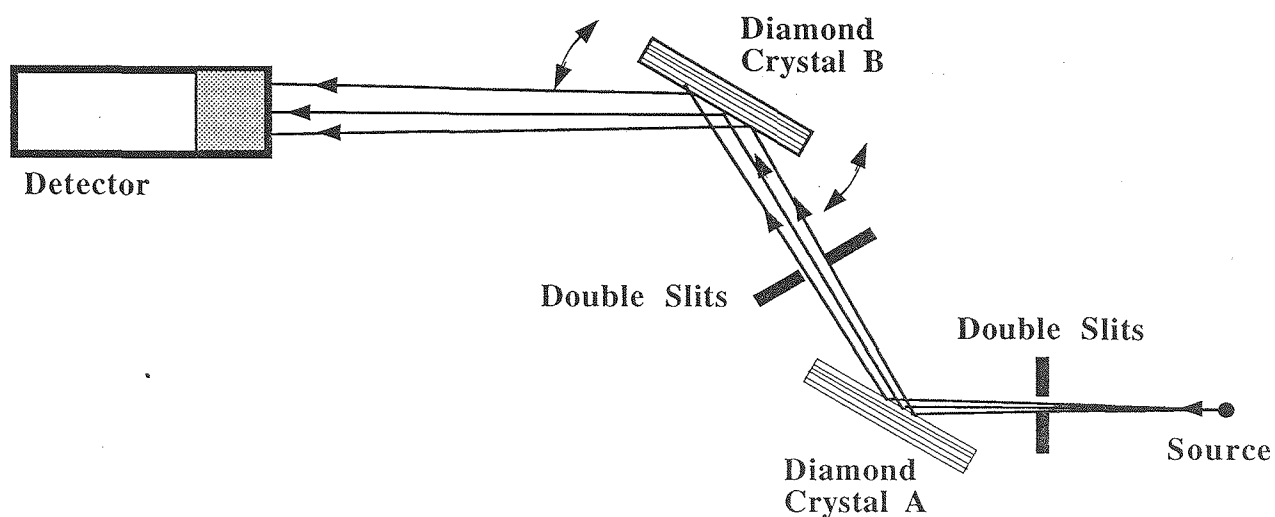


Figure 1. Experimental setup (viewed from the top) for the rocking curve measurements. The x-ray beam from the Mo x-ray source on the right passes through a set of double slits and is incident on the Crystal A. Crystal A diffracts the $K\alpha_1$ x-ray line, which passes through the second set of double slits and is diffracted a second time by the Crystal B. The final intensity is detected in the detector on the left.

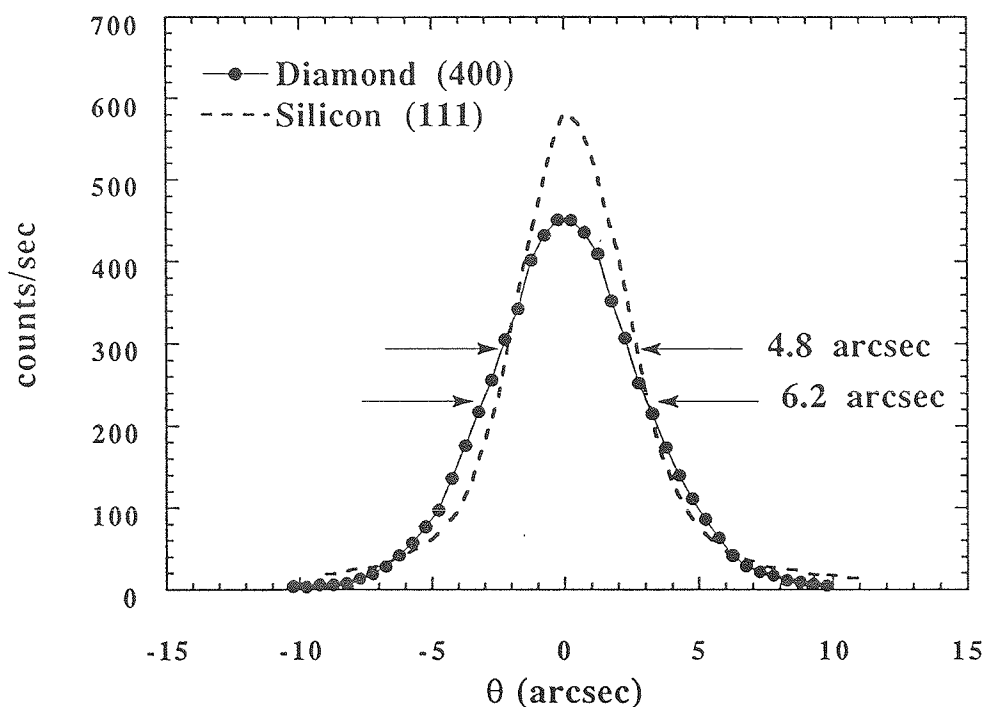


Figure 2. Double crystal rocking curves for the synthetic diamond (400) and silicon (111) crystals with the Mo $K\alpha 1$ x-ray. The counting rate in the detector is plotted versus the Bragg diffraction angle of the second crystal using an arbitrary zero located near the center of the peak.

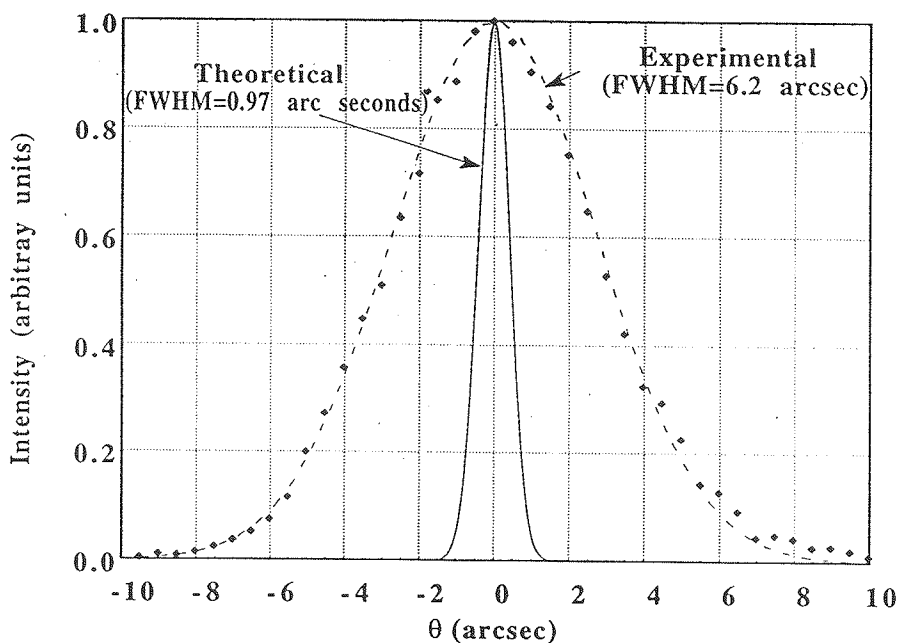


Figure 3. Comparison of the measured and theoretical double crystal rocking curves of diamond (400) using photons from Mo $K\alpha 1$.

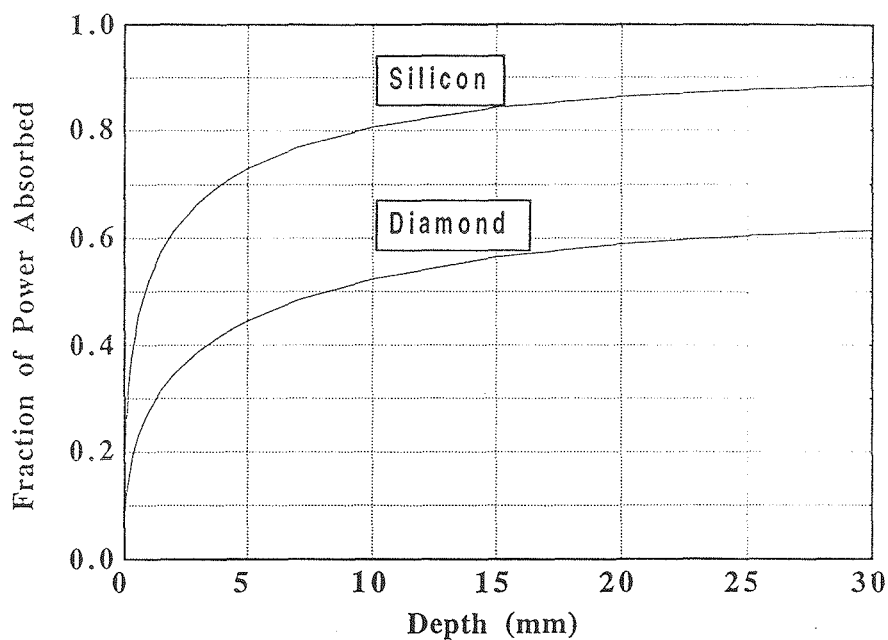


Figure 4. The absorption of the APS Undulator A beam in diamond and silicon computed from a bending magnet approximation for the source with a characteristic energy of 23.5 keV.

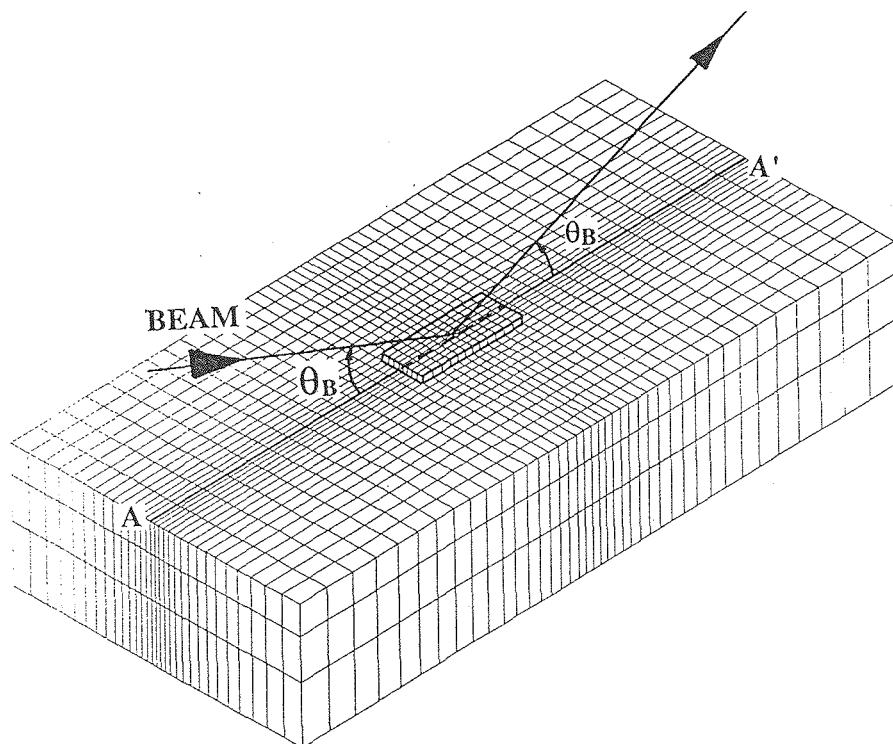


Figure 5. The monochromator model used in the analysis of the diamond monochromator. The substrate is CVD diamond while the diffracting element bonded to it is single crystal diamond shown in heavy lines.

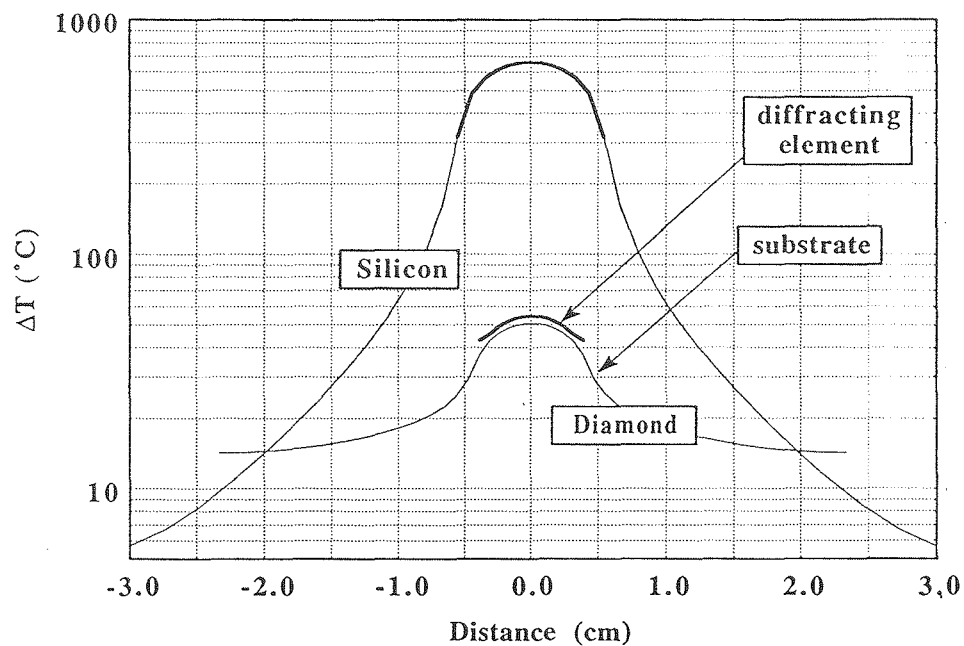


Figure 6. Temperature rise in the 1-cm-thick silicon and diamond crystals along the AA'-axis of Fig. 5.

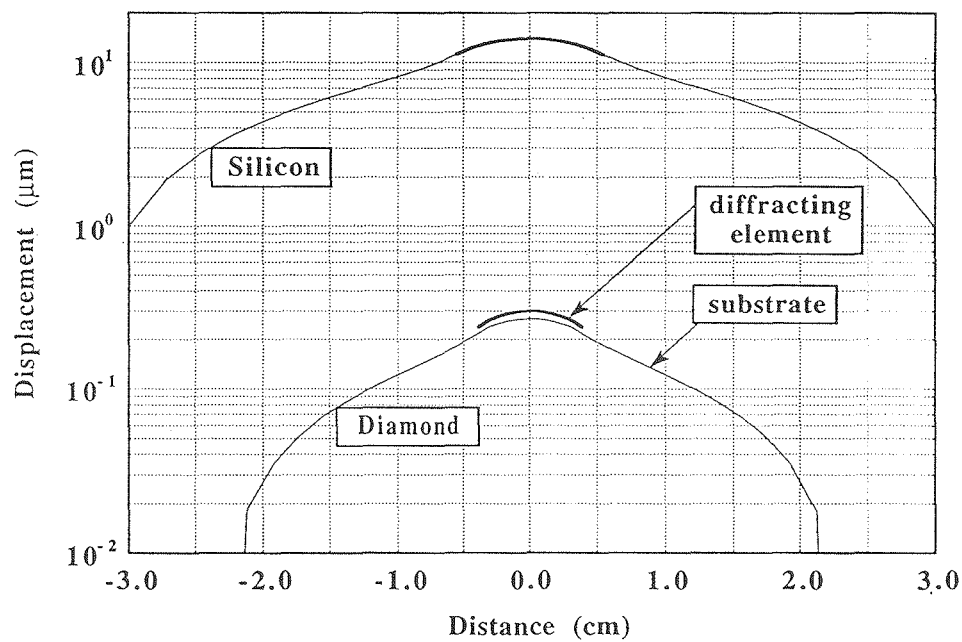


Figure 7. The displacement along the AA'-axis of Figure 5 in the 1-cm-thick silicon and diamond crystals under the APS undulator beam at closed gap.

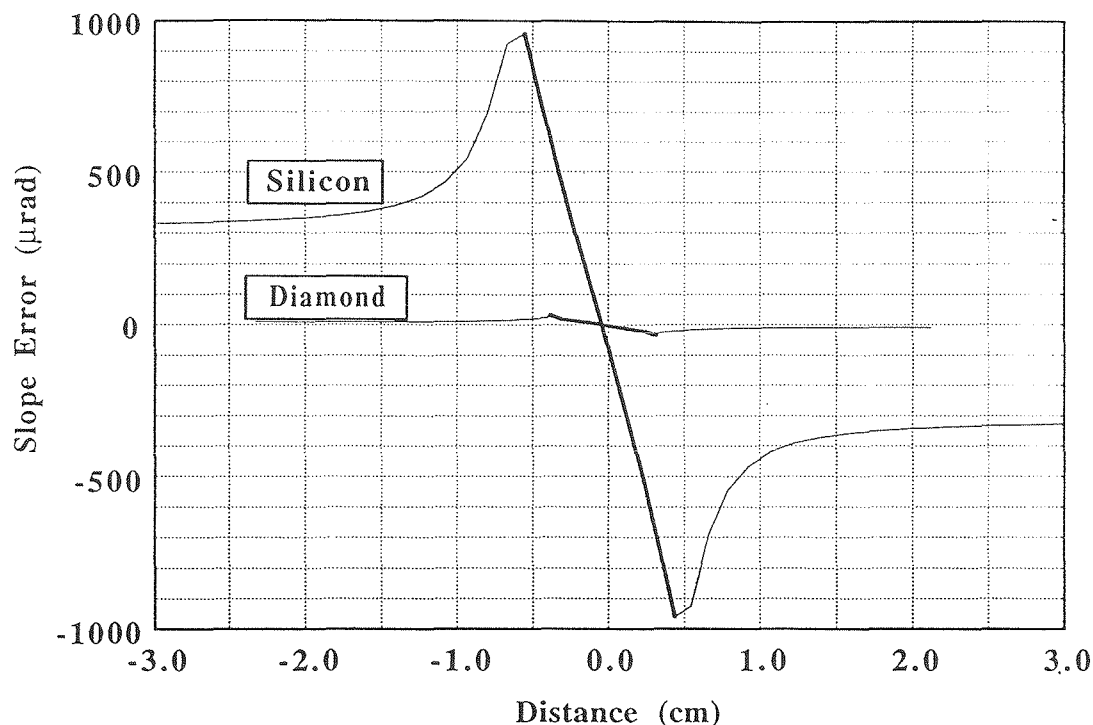


Figure 8. Slope errors along the AA'-axis of Figure 5 for the silicon and diamond crystals under the APS Undulator beam at closed gap.

8. ACKNOWLEDGMENTS

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